Urea, (m-fluorophenyl)-770-19-4 | DTXSID40227815

Model Performance

| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (| Training (75%) | | Test (25%) | |
|-----------------|------|------------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 | |

Model Results

Predicted value: 250 °C

Global applicability domain: Outside

Local applicability domain index: 2.20e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

Image not found

1-Phenylurea Measured: 238 Predicted: 247

Image not found

N-(4-Bromophenyl)urea Measured: 260 Predicted: 256

Image not found

1,3-Dipropylurea Measured: 255 Predicted: 256

Image not found

Urea, N,N'-diethyl (9CI) Measured: 263 Predicted: 262

Image not found

N,N'-Dimethylurea Measured: 269 Predicted: 267